Spontaneous formation of a π soliton in a superconducting wire with an odd number of electrons

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We consider a one-dimensional superconducting wire where the total number of electrons can be controlled in the Coulomb blockade regime. We predict that a π soliton (kink) will spontaneously form in the system when the number of electron is odd, because this configuration has a lower energy. If the wire with an odd number of electrons is closed in a ring, the phase difference on the two sides of the soliton will generate a supercurrent detectable by SQUID. The two degenerate states with the current flowing clockwise or counterclockwise can be utilized as a qubit.

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Introduction. In a mesoscopic sample in the Coulomb blockage regime, the total number of electrons can be controlled discretely by gate voltage [1]. It was predicted theoretically [2] and verified experimentally [3] that the ground-state energies of a superconducting sample with even and odd number of electrons differ by the superconducting gap Δ_0, because the odd electron cannot form a Cooper pair. In the present paper, we discuss another manifestation of the even-odd asymmetry in a one-dimensional (1D) superconducting wire or constriction. We show that when such a system has an odd number of electrons, it can lower its energy by spontaneously forming a kink soliton of the order parameter, analogously to the charge-density-wave solitons in polyacetylene [4, 5, 6] and other systems with similar broken symmetry [7]. If the wire is closed in a ring, the phase difference on the two sides of the soliton would produce a supercurrent in the ring, which could be detected by a sensitive SQUID. The two degenerate states with the current flowing clockwise or counterclockwise can be considered as a qubit [8].

1D superconductor with a kink soliton. Let us consider a 1D s-wave BCS superconductor characterized by the mean-field Hamiltonian density

$$\hat{H}(x) = \hat{c}_\uparrow^\dagger(x)\,\hat{\xi}\,\hat{c}_\uparrow(x) + \hat{c}_\downarrow^\dagger(x)\,\hat{\xi}\,\hat{c}_\downarrow(x) \qquad (1)$$
$$+\,\hat{c}_\downarrow(x)\,\Delta^*(x)\,\hat{c}_\uparrow(x) + \hat{c}_\uparrow^\dagger(x)\,\Delta(x)\,\hat{c}_\downarrow^\dagger(x) - |\Delta(x)|^2/g.$$

Here $\hat{c}^{(\dagger)}_{\uparrow,\downarrow}(x)$ are the creation and destruction operators of electrons with the spin projections $\uparrow$ and $\downarrow$ at the point x, $\Delta(x)$ is the superconducting pairing potential satisfying the self-consistency condition $\Delta(x) = g\langle\hat{c}_\downarrow(x)\hat{c}_\uparrow(x)\rangle$, $g<0$ is the BCS coupling constant, and $\hat{\xi}$ is the kinetic energy operator. Near the Fermi energy, the electron dispersion relation can be linearized: $\hat{\xi} \approx -\alpha i v_F\partial_x$, where $\alpha = \pm$ labels the right- and left-moving electrons with the momenta near the two Fermi points αk_F, v_F is the Fermi velocity, and the Planck constant is $\hbar = 1$. All calculations in the paper are done at zero temperature.

The eigenstates of Hamiltonian (1) are the Bogoliubov quasiparticles characterized by the wave functions $\psi_n^{(\alpha)}(x) = [u_n^{(\alpha)}(x), v_n^{(\alpha)}(x)]$ that satisfy the Bogoliubov-de Gennes (BdG) equation [9]

$$\begin{pmatrix} -\alpha i v_F\partial_x & \Delta(x) \\ \Delta^*(x) & \alpha i v_F\partial_x \end{pmatrix}\psi_n^{(\alpha)}(x) = E_n^{(\alpha)}\psi_n^{(\alpha)}(x) \qquad (2)$$

with the eigenenergies $E_n^{(\alpha)}$. The spectrum of Eq. (2) consists of solutions with positive and negative energies related by charge conjugation. The superconducting ground-state energy F relative to the normal state energy and the BCS self-consistency relation can be expressed in terms of these solutions [9]:

$$F = \sum_{n,\alpha}\left(E_n^{(\alpha)} + |\xi_n^{(\alpha)}|\right) - \int dx\,|\Delta(x)|^2/g, \qquad (3)$$
$$\Delta(x) = -g\sum_{n,\alpha} u_n^{(\alpha)}(x)\,v_n^{(\alpha)*}(x), \qquad (4)$$

where the sums are taken over the occupied states with $E_n^{(\alpha)} < 0$.

Suppose the pairing potential has a phase soliton (kink) at $x=0$, so that $\Delta(x)\to\Delta_0 e^{\pm i\phi}$ at $x\to\pm\infty$:

$$\Delta(x) = \Delta_1 + i\Delta_2(x), \quad \Delta_1 = \Delta_0\cos\phi, \qquad (5)$$
$$\Delta_2(x) = \kappa v_F\tanh\kappa x, \quad \kappa = \Delta_0\sin\phi/v_F. \qquad (6)$$

In this case [10, 11], the spectrum of Eq. (2) has a continuous part $\pm E_q^{(\alpha)}$, where q is the quasiparticle momentum counted from αk_F, and discrete subgap states $E_0^{(\alpha)}$:

$$E_q^{(\alpha)} = \sqrt{(v_F q)^2 + \Delta_0^2}, \quad E_0^{(\alpha)} = -\alpha\Delta_0\cos\phi. \qquad (7)$$

The energies $E_0^{\pm}(\phi)$ of the subgap states (7) are shown in Fig. 1(a) by the thick solid and dashed lines. The total energy F, given by Eq. (3), can be separated into the contributions from the continuous spectrum and from the discrete states. The former contribution, counted from the ground state energy of a uniform BCS superconductor with an even number of electrons, has the form

$$F_c = \Delta_0 - 2\sum_{q_j}\left(E_{q_j} - E_{\bar{q}_j}\right) - \int dx\,\frac{|\Delta(x)|^2 - \Delta_0^2}{g}. \qquad (8)$$

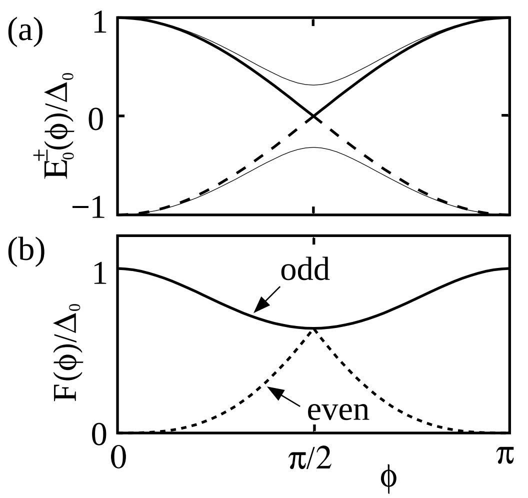

FIG. 1: (a) The energies $E_0^{(\alpha)}$ of the subgap bound states vs phase ϕ. The thick solid and dashed lines correspond to the transmission coefficient $\tau = 1$, and the thin lines to $\tau = 0.9$. (b) The total energy F of the one-channel superconducting wire with an odd (solid line) and an even (dashed line) number of electrons vs phase ϕ, calculated for $\tau = 1$.

The first term in the r.h.s. of Eq. (8) reflects the fact that one state has been removed from the continuum to the discrete spectrum. The factor 2 in front of the second term represents the equal contributions from the states with $\alpha = \pm$. In the second term, $q_j = \bar{q}_j - \zeta_j/L$ is the quasiparticle momentum displaced by the phase shift ζ_j from the unperturbed value $\bar{q}_j = 2\pi j/L$ for a uniform system without a kink. (Here the periodic boundary condition over the length L is implied, and j is an integer.) The calculations of the phase shifts and the dependence of F_c on ϕ are given at the end of the paper (see also [4, 5, 12]). The result is

$$F_c(\phi) = \frac{2\Delta_0}{\pi}\left[\left(\frac{\pi}{2} - \phi\right)\cos\phi + \sin\phi\right]. \tag{9}$$

Let us examine how the ground state energies $F_e(\phi)$ and $F_o(\phi)$ of the system with an even and an odd number of electrons depend on the phase difference 2ϕ. At $\phi = 0$, the spectrum has only the continuous part, which is completely filled below $-\Delta_0$ and completely empty above $+\Delta_0$ when the number of electrons is even. As ϕ increases, the discrete state (7) with the negative energy remains occupied, whereas the one with the positive energy is empty. Thus,

$$F_e(\phi) = F_c(\phi) - \Delta_0|\cos\phi|. \tag{10}$$

As shown in Fig. 1(b) by the dashed line, $F_e(\phi)$ is minimal at $\phi = 0$. Thus, the system with an even number of electrons prefers a uniform state.

On the other hand, when the number of electrons is odd, the quasiparticle state with the energy $+\Delta_0$ is filled by the odd electron at $\phi = 0$ [2]. Thus, as ϕ increases, both the lower and upper discrete states (7) stay occupied. Because their energies cancel, the total energy in the odd case is

$$F_o(\phi) = F_c(\phi), \tag{11}$$

which is shown by the solid line in Fig. 1(b). In contrast to the even case, $F_o(\phi)$ decreases with increasing ϕ and has a minimum at $\phi = \pi/2$ with the energy $E_s = F_o(\pi/2) = 2\Delta_0/\pi < \Delta_0$, lower than in the uniform state. Thus, a 1D superconductor with an odd number of electrons should spontaneously create a kink with the phase difference $2\phi = \pi$ in order to decrease the total energy. This phenomenon is analogous to creation of a soliton in a charge- or spin-density wave with an odd number of electrons [4, 5, 6, 7].

Now let us consider the case where the 1D superconducting wire has N channels, e.g. consists of N parallel chains with the common potential $\Delta(x)$. When the number of electrons is odd, N discrete states with negative energies (7) and one with positive energy are filled. So, the total energy of the system is $F_o(\phi) = NF_c(\phi) - (N-1)\Delta_0|\cos\phi|$, and the minimum $(\Delta_0 2N/\pi)\sin(\pi/2N)$ is achieved at $2\phi = \pi/N$. Thus, the soliton also forms in this case, but with the phase difference reduced by $1/N$. When $N \gg 1$, the energy gain is insignificant, and soliton formation becomes irrelevant.

Superconducting ring with a kink. Now suppose that the 1D superconducting wire (with $N = 1$) is closed in a ring of length L. The length L is assumed to be much longer than the coherence length $\xi = \hbar v_F/\Delta_0$, so the soliton energy E_s is not significantly affected by closing of the wire. On the other hand, L should be short enough, so that the whole ring is in the Coulomb blockade regime, and an external gate can control the total number of electrons to be odd. The latter condition requires that $\Delta_0 < E_c$ [2], where $E_c \sim e^2/D$ is the Coulomb charging energy, and D is the overall size of the sample. For a simple ring, $D = L$, but in general $D \gtrsim L$, as discussed below. Thus, we need

$$\xi = \hbar v_F/\Delta_0 \ll L \lesssim D \lesssim e^2/\Delta_0, \tag{12}$$

so the Fermi velocity has to be much lower than the Bohr velocity: $v_F \ll e^2/\hbar = 2.2 \times 10^8$ cm/s. This condition is satisfied in a typical metal with $v_F \sim 10^7$ cm/s.

When the number of electrons is odd, the soliton creates the phase difference $2\phi = \pi$ between the ends of an open wire. However, when the wire is closed, the superconducting phase θ must continuously interpolate between the phases $\pm\pi/2$ at the opposite sides of the soliton, so $\Delta(x) = \Delta_0 e^{i\theta(x)}$. The small phase gradient $|\partial\theta/\partial x| = \pi/L$ creates the supercurrent

$$J = \pm\frac{en_s}{2m}\frac{\partial\theta}{\partial x} = \pm\frac{ev_F}{L}, \tag{13}$$

where $n_s = 4k_F/2\pi$ is the superfluid density equal to the total electron density at zero temperature [13]. Notice

that the supercurrent J can flow in the ring either clockwise or counterclockwise, thus the time-reversal symmetry is spontaneously broken. These two degenerate states can be viewed as a qubit [8]. The supercurrent (13) is equal to the maximal persistent current in a normal (nonsuperconducting) ring with an odd number of electrons [14]. It corresponds to the odd electron of charge e moving with the Fermi velocity v_F around the ring of circumference L. This current creates the magnetic flux $\Phi \sim JL/c \sim ev_F/c \sim 10^{-5}\Phi_0$ (where $\Phi_0 = \pi\hbar c/e$ is the flux quantum), which could be detected, in principle, by a sensitive SQUID. *We predict that, when the number of electrons in the ring is switched between odd and even by an external gate, the current (13) should appear and disappear in the ring.* In the case of N channels, the current is given by the same Eq. (13).

Above we considered an idealized situation of a uniform superconducting ring. However, the conclusion also applies to other, more realistic experimental setups. Suppose a straight 1D superconducting wire of length L, e.g. a carbon nanotube [15], is shunted by a thick conventional superconductor of size D. In this case, the soliton and the phase gradient are localized within the 1D wire, whereas the phase gradient over the shunt is close to zero, so the supercurrent is given by Eq. (13). Another setup is a narrow constriction with a small number N of conducting channels in a thick superconducting ring. In this case, L is the length of the 1D constriction, and D is the overall size of the ring. In general, when the ring is nonuniform, the transmission coefficient τ through the weak link is less than one. In this case, the energies of the subgap states are $E_0 = \pm\Delta_0\sqrt{1-\tau\sin^2\phi}$ [10, 11], shown by the thin lines in Fig. 1(a). Although we cannot calculate $F_c(\phi)$ exactly when $\tau \neq 1$, the total energy of the system should be close to Eq. (9) if $\tau \approx 1$, and the kink soliton should be still energetically favorable. Thus, our theory should be applicable to the atomic contacts with $N \sim 1$ and $\tau \approx 1$ realized in experiments [16].

Calculation of $F_c(\phi)$ via phase shifts. To simplify presentation, we write the equations below specifically for $\alpha = +$. In order to calculate the phase shifts, let us introduce the wave functions $f_\pm(x) = u(x) \pm v(x)$. (Notice that this index $\pm$ is different from α.) Then the BdG equation (2) acquires the supersymmetric form [17, 18]

$$(E \mp \Delta_1) f_\pm = -iv_F\,\partial f_\mp/\partial x \mp i\Delta_2(x) f_\mp, \quad (14)$$

$$\left(E^2 + v_F^2\,\frac{\partial^2}{\partial x^2} - |\Delta(x)|^2 \mp v_F\,\frac{\partial \Delta_2(x)}{\partial x}\right) f_\pm = 0. \quad (15)$$

Substituting Eqs. (5) and (6) into Eqs. (14) and (15), we find the (unnormalized) wave functions

$$f_+(x) = e^{iqx}, \quad f_-(x) = \frac{v_F q + i\Delta_2(x)}{E+\Delta_1} e^{iqx}. \quad (16)$$

From Eq. (16), we observe that, when x changes from $-\infty$ to $+\infty$, f_- acquires the phase factor $\Xi = (q + i\kappa)/(q - i\kappa)$. In order to impose periodic boundary conditions consistently, let us assume that the system also has an antikink far away from $x = 0$. In a similar manner, it is easy to show that f_+ acquires the same phase factor Ξ upon traversing the antikink. Thus, when x changes from one boundary of the sample to another, both $f_\pm$ experience the phase shift $\zeta_q = \arctan(\kappa/q)$ per *one* soliton [5, 12]. The same result can be also obtained by imposing zero boundary conditions at the ends of the wire.

Using the relation $q_j = \bar{q}_j - \zeta_j/L$, we write Eq. (8) as

$$F_c = \Delta_0 + 2\int \frac{dq}{2\pi}\,\zeta_q\,\frac{\partial E_q}{\partial q} + \frac{2\kappa v_F^2}{g}, \quad (17)$$

where we took the integral over x using Eqs. (5) and (6). Integrating by parts over q and taking into account the BCS self-consistency relation

$$-\frac{1}{g} = \int \frac{dq}{2\pi E_q}, \quad (18)$$

we rewrite Eq. (17) as follows

$$F_c = \frac{2v_F\kappa}{\pi} - 2\int \frac{dq}{2\pi}\left(E_q\,\frac{\partial \zeta_q}{\partial q} + \frac{v_F^2\kappa}{E_q}\right). \quad (19)$$

Substituting $\zeta_q = \arctan(\kappa/q)$ into Eq. (19) and taking the integral over q, as in Ref. [12], we obtain Eq. (9).

An alternative calculation of $F_c(\phi)$. Following the method of Ref. [4], let us calculate the derivative

$$\frac{dF_c(\phi)}{d\phi} = \int dx\left[\frac{\delta F_c}{\delta \Delta^*(x)}\frac{\partial \Delta^*(x)}{\partial \phi} + \text{c.c.}\right]. \quad (20)$$

We write the eigenenergies of the BdG equation (2) as

$$E_n^{(\alpha)} = \int dx\,[u_n^{(\alpha)*}(x)\,\hat{\xi}\,u_n^{(\alpha)}(x) - v_n^{(\alpha)}(x)\,\hat{\xi}\,v_n^{(\alpha)*}(x) + u_n^{(\alpha)}(x)\,\Delta^*(x)\,v_n^{(\alpha)*}(x) + v_n^{(\alpha)}(x)\,\Delta(x)\,u_n^{(\alpha)*}(x)], \quad (21)$$

where the normalization condition $\int dx(|u|^2 + |v|^2) = 1$ is implied. Taking variational derivatives of Eqs. (8) and (21) with respect to $\Delta^*(x)$, we find

$$\frac{\delta F_c}{\delta \Delta^*(x)} = -\sum_{q,\alpha} u_q^{(\alpha)}(x)\,v_q^{(\alpha)*}(x) - \frac{\Delta(x)}{g}. \quad (22)$$

The normalized wave functions $\psi_q^{(\alpha)} = (u_q^{(\alpha)}, v_q^{(\alpha)})$ can be deduced from Eq. (16)

$$\psi_q^{(\alpha)} = \sqrt{\frac{E_q + \alpha\Delta_1}{4LE_q}}\begin{pmatrix} 1 + \alpha\frac{v_F q + i\Delta_2(x)}{E_q + \alpha\Delta_1} \\ \alpha - \frac{v_F q + i\Delta_2(x)}{E_q + \alpha\Delta_1}\end{pmatrix} e^{iqx}. \quad (23)$$

Using Eq. (23), we find

$$\sum_{q,\alpha} u_q^{(\alpha)} v_q^{(\alpha)*} = \Delta(x)\int \frac{dq}{2\pi E_q} - \frac{\kappa(\pi/2 - \phi)}{2\pi\cosh^2(\kappa x)}. \quad (24)$$

where the summation over q_j has been simply replaced by integration over q, because the phase shifts contribute only a negligible term proportional to $1/L$. Substituting Eq. (24) into Eq. (22) and using Eq. (18), we find

$$\frac{\delta F_c}{\delta \Delta^*(x)} = \frac{\kappa(\pi/2-\phi)}{2\pi\cosh^2(\kappa x)}. \tag{25}$$

Substituting Eq. (25) and $\partial\Delta^*/\partial\phi$ determined from Eqs. (5) and (6) into Eq. (20) and integrating over x, we get

$$\frac{dF_c}{d\phi} = -\frac{2\Delta_0}{\pi}\left(\frac{\pi}{2}-\phi\right)\sin\phi. \tag{26}$$

Integrating Eq. (26) over ϕ, we recover Eq. (9).

We can also check that the self-consistency condition (4) is satisfied at $\phi = \pi/2$. Indeed, the last term in the r.h.s. of Eq. (24) vanishes, and the first term gives $-\Delta(x)/g$ because of Eq. (18), whereas the contributions of the localized states

$$\psi_0^{(\alpha)}(x) = \frac{\sqrt{\kappa}}{2\cosh\kappa x}\begin{pmatrix} 1 \\ -\alpha \end{pmatrix} \tag{27}$$

mutually cancel for $\alpha = \pm$.

Conclusions. We have shown that a 1D superconducting wire with an odd number of electrons can lower its energy by creating a π soliton (kink) of the order parameter, so that the odd unpaired electron occupies the midgap bound state localized at the soliton. In order to exhibit this effect, the wire does not have to be completely uniform. It is sufficient that it has a 1D portion with the length L longer than the coherence length ξ and the atomic-size cross-section with the number of conducting channels $N \sim 1$ and the transmission coefficient $\tau \approx 1$. Such atomic Josephson contacts have been already realized experimentally [16]. Another possibility is to use a carbon nanotube [15].

If the wire is closed in a ring, the phase difference on the two sides of the soliton would generate a supercurrent in the ring, which could be detected by a sensitive SQUID. The total number of electrons in the ring can be controlled by an external gate in the Coulomb blockade regime. *We predict that the supercurrent should appear in the ring when the number of electrons is odd and disappear when the number is even.* The current can flow either clockwise or counterclockwise. These two degenerate states can be viewed as a qubit and utilized for quantum computing [8].

Spontaneous current in a ring with phase circulation π was recently predicted for unconventional superconductors using exotic theory of fractional spin-charge separation [19] and was disproved experimentally [20]. That theory did not consider the difference between even and odd number of electrons or the setup with only one or few conducting channels. These mesoscopic aspects play crucial role in our theory, which is formulated completely within the conventional BCS framework.

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[1] D. V. Averin and K. K. Likharev, in *Mesoscopic Phenomena in Solids*, edited by B. L. Altshuler, P. A. Lee, and R. A. Webb (Elsevier, Amsterdam, 1991); *Single Charge Tunneling*, edited by H. Grabert and M. H. Devoret (Plenum, New York, 1992).

[2] D. V. Averin and Y. V. Nazarov, Phys. Rev. Lett. **69**, 1993 (1992).

[3] M. T. Tuominen *et al.*, Phys. Rev. Lett. **69**, 1997 (1992); P. Lafarge *et al.*, Phys. Rev. Lett. **70**, 994 (1993).

[4] S. A. Brazovskii, Zh. Eksp. Teor. Fiz. **78**, 677 (1980) [Sov. Phys. JETP **51**, 342 (1980)].

[5] H. Takayama, Y. R. Lin-Liu, and K. Maki, Phys. Rev. B **21**, 2388 (1980).

[6] A. J. Heeger, S. Kivelson, J. R. Schrieffer, and W.-P. Su, Rev. Mod. Phys. **60**, 781 (1988).

[7] S. A. Brazovskii, in *Electronic Correlations: From Meso- to Nano-Physics*, edited by T. Martin, G. Montambaux, and J. Trân Thanh Vân (EDP Sciences, France, 2001).

[8] C. P. Williams and S. H. Clearwater, *Explorations in Quantum Computing* (Springer, New York, 1998).

[9] P. G. de Gennes, *Superconductivity of Metals and Alloys* (Addison-Wesley, New York, 1989); M. Tinkham, *Introduction to Superconductivity* (McGraw-Hill, New York, 1996).

[10] A. Furusaki and M. Tsukada, Physica B **165**&**166**, 967 (1990); Phys. Rev. B **43**, 10164 (1991); C. W. J. Beenakker, Phys. Rev. Lett. **67**, 3836 (1991).

[11] D. A. Ivanov and M. V. Feigel'man, Zh. Eksp. Teor. Fiz. **114**, 640 (1998) [Sov. Phys. JETP **87**, 349 (1998)]; Phys. Rev. B **59**, 8444 (1999); D. V. Averin, Phys. Rev. Lett. **82**, 3685 (1999).

[12] R. F. Dashen, B. Hasslacher, and A. Neveu, Phys. Rev. D **12**, 2443 (1975).

[13] In the presence of the supercurrent (13), the phase difference 2ϕ of the kink slightly deviates from π producing the current $J = \partial F(\phi)/\partial\phi$ through the kink [10, 11], which is necessary to maintain current continuity. However, this small deviation does not affect the soliton energy E_s significantly if $L \gg \xi$.

[14] H.-F. Cheung *et al.*, Phys. Rev. B **37**, 6050 (1988).

[15] Z. K. Tang *et al.*, Science **292**, 2462 (2001); M. Kociak *et al.*, Phys. Rev. Lett. **86**, 2416 (2001).

[16] M. F. Goffman *et al.*, Phys. Rev. Lett. **85**, 170 (2000); E. Scheer *et al.*, *ibid.* **86**, 284 (2001); R. Cron *et al.*, *ibid.* **86**, 4104 (2001).

[17] F. Schwabl, *Quantum Mechanics* (Springer, Berlin, 1995) Ch. 19; G. Junker, *Supersymmetric Methods in Quantum and Statistical Physics* (Springer, Berlin, 1996).

[18] I. Kosztin, Š. Kos, M. Stone, and A. J. Leggett, Phys. Rev. B **58**, 9365 (1998); I. Adagideli, P. M. Goldbart, A. Shnirman, and A. Yazdani, Phys. Rev. Lett. **83**, 5571 (1999).

[19] T. Senthil and M. P. A. Fisher, Phys. Rev. Lett. **86**, 292 (2001); Phys. Rev. B **63**, 134521 (2001).

[20] D. A. Bonn *et al.*, Nature **414**, 887 (2001).